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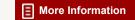
Fostering Increased Cooperation Between the Geological and Materials Sciences (1982)

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↑ Fostering Increased Cooperation Between the Geological And Materials Sciences

Committee on Geological and Materials Sciences
Commission on Physical Sciences,
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PREFACE

This report is written with the hope of stimulating new and further interaction between research scientists in the earth and the materials sciences. Workers in these fields often study the same natural phenomena and use similar instruments. The chief differences are the actual substances used in the experiments, and, sometimes, the questions that are being asked of nature. In general, the earth scientist is studying the structure and composition of natural materials to find out how the earth has been formed; the materials scientist is studying the structure and composition of both natural and processed materials so as to control their properties and behavior.

The overall similarity of methods and instruments used suggests that frequent interchange between the two fields would be mutually profitable. Indeed, such interchange, when it has occurred, has been beneficial.

In October 1976, the Advisory Board of the Office of Earth Sciences considered, as an item on its agenda, the desirability and benefits of more direct interaction between the geological sciences and other branches of science and engineering. The discussion resulted in a proposal to convene an ad hoc meeting of scientists and engineers from the geological sciences and materials science under the auspices of the Assembly of Mathematical and Physical Sciences (now the Commission on Physical Sciences, Mathematics, and Resources: CPSMR). The purpose was to determine (1) the extent to which these sciences would benefit from increased interaction, (2) the best methods for improving interaction, e.g., studies and/or conferences, and (3) the objectives for any recommended action.

An ad hoc committee from academia, government, and industry was appointed in February 1978, and it met on April 28, 1978, at the headquarters of the Geological Society of America in Boulder, Colorado. The committee considered the following questions:

- (a) Is there much to be gained by more interaction between workers from these two communities?
- (b) If the answer to (a) is yes, what would be the best way to accomplish this interaction?
- (c) Should the interaction be in the form of organized entities, e.g., cooperative studies, conferences, workshops? Or should it be informal, relying on individual contacts?
- (d) What should be done to foster interactions between these and other related areas?

The consensus of the committee was that increased interaction would indeed facilitate more rapid transfer of data, concepts, and instrumentation. This transfer could be expected to contribute in turn to more expeditious solutions of important national problems in addition to benefiting both sets of disciplines through advances in our level of knowledge. A benefit that would accrue as a by-product would be the formation of a more diversified pool of trained manpower and facilities, which could then be drawn upon in solving the next generation of problems. Increased interaction and cooperation should accelerate progress in solving many of the technological problems that we face today.

Out of the meeting in Boulder came the further recommendation that an ad hoc committee be established in the National Research Council to devise new means to stimulate interaction between the geological and materials sciences, to oversee the performance of several important tasks

by smaller ad hoc groups, and to serve as a focal point for information transfer. This committee was to have a lifetime of at least a few years and was to consist of members drawn jointly from CPSMR and what was then the Assembly of Engineering, now the Commission on Engineering and Technical Systems. Further, its membership was to adequately represent both the geological and the materials sciences communities. The tasks to be undertaken by the ad hoc groups were to be carried out in cooperation with other National Research Council groups, with government organizations, with industry, and with professional societies when possible. The first tasks to be undertaken by these groups were to include the following:

- 1. To identify and help remove or minimize impediments to effective interdisciplinary interactions within universities, industry, and government agencies.
- 2. To examine the mechanisms through which basic interdisciplinary research needs are incorporated into long-range planning for major projects in the geosciences.
- To examine the need for regional and/or national centers that could provide special facilities.
- 4. To foster interactions between geoscientists and materials scientists through the medium of conferences at which attendees would be drawn from diverse traditional disciplines.
- 5. To complement the workshops with lecture series, symposiums, and similar events that would bring together more of the rank and file of the two fields (including graduate students) who do not have a preexisting common interest.

INTRODUCTION

This report is concerned with areas of overlap between two large, diverse, and dynamic fields -- the geological and the materials sciences -- and specifically with the kinds of research carried out by investigators in the two fields. As noted in the preface, the Committee on Geological and Materials Sciences, formed under the former Assembly of Mathematical and Physical Sciences (now the Commission on Physical Sciences, Mathematics, and Resources) of the National Research Council, had a primary goal of exploring how the nation could benefit from increased cooperation and exchange of information between the two fields. Because of the nature of the founding body and the makeup of the committee, more emphasis was placed on how the geological sciences could be made more effective through the transfer of theories and techniques from materials science rather than on how the geological sciences could benefit materials science, although some important examples of the latter were also identified and discussed by the committee. From the first meeting, it was apparent that we were dealing with a large area of activity, from basic research to processing of materials, and from the university environment to industrial production. Accordingly, we felt that we should concentrate on problems of basic research, education, and transfer of information, with the idea that progress would have to be made in these areas before we could hope to have an impact on industry, the larger independent research institutions, or mission-oriented government agencies.

Although there has been no recent precise survey, the American Geological Institute estimates the number of practicing earth scientists, (i.e., those with academic training and who are working in geology,

geochemistry, or geophysics) at greater than 50,000. Of these, however, we estimate that only 2000 to 3000 are involved in research on the properties of geological materials or the application of that research. The field of materials science is much larger and harder to define because it encompasses activities related to almost all scientific and engineering disciplines.

According to a recent survey sponsored by the U.S. Department of Commerce/National Bureau of Standards (COMAT Committee Report, 1981), the total amount of money spent by federal agencies on materials R&D in 1980 was \$1,103,683,000. This was about equally divided between basic research, applied research, and development. We cannot be sure just what is included, but it probably represents a very broad view of materials research. No comparable figures are available for money spent on the properties of geological materials, but it can safely be assumed to be on the order of 100 times less. A better comparison can be made for basic research supported by the National Science Foundation (NSF). In 1980, the budget of the NSF Division of Materials Research was \$68,715,551, whereas the amount spent on geological materials from the budget of the Division of Earth Sciences was estimated to have been about \$4,000,000 out of a total Division budget of \$25,982,722.

We conclude from these figures that research on geological materials constitutes only a small fraction of the total materials effort.

Therefore it is not surprising that most advances in scientific theory and most developments in experimental techniques and apparatus take place in the broader area of materials science. Nevertheless, national R&D efforts on earth materials are of great importance because of the vital need for discovery and exploitation of ore deposits, for improved methods

of recovery of elements and compounds from ores, and for dealing with the complex environmental problems associated with all aspects of the materials cycle.

It should also be noted that the loci of principal research in the two fields are different. Major developments and progress in materials science research take place in industrial laboratories, with universities playing a subordinate role. The opposite is true for the geosciences.

Creation of materials research groups at several universities by the Advanced Research Projects Agency (ARPA), beginning some twenty years ago, has strengthened materials programs at some universities; and geoscience research by industry made great strides as oil companies developed excellent research programs. Nevertheless, in general the cutting edge for materials research remains in industry, and for geoscience research it is in academic institutions. This situation suggests that the greatest benefits could be expected by increased communication and cooperative research between university geoscience research groups and industrial materials laboratories. There is a trend in this direction, as research projects are being established at universities when funding is by a group of companies and is intended to continue for several years. This effort needs to be expanded.

THE MATERIALS CYCLE

Figure 1 illustrates the areas in the materials cycle in which geological and materials scientists are primarily involved. The geological scientists are interested in the exploration for mineral

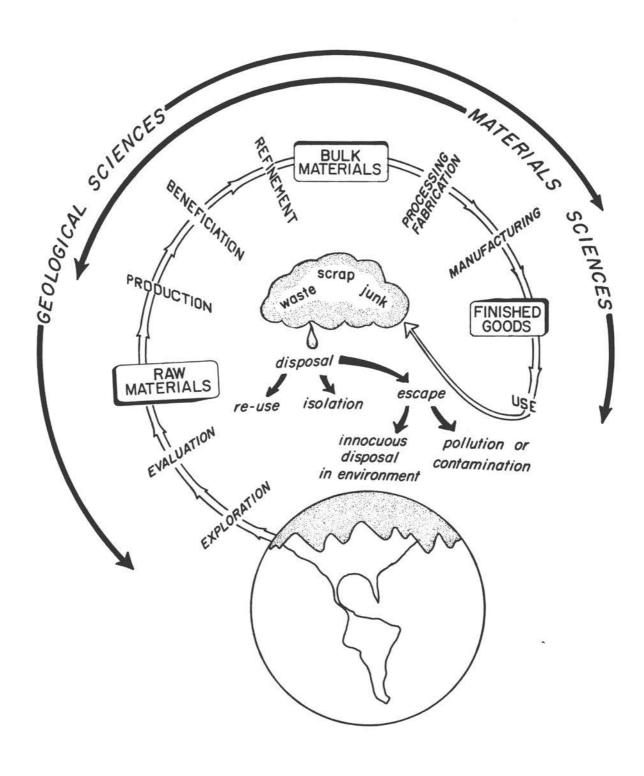


FIGURE 1 The materials cycle.

resources and their production, and in the processes through which bulk materials are obtained from raw materials. Materials scientists play their important role in the various stages that lead to finished goods and, eventually, to disposal of junk and waste material. Geological scientists again become involved at this latter stage and have an important role in the problems relating to the disposal and dispersal of unwanted products. In time, both groups of scientists will have an ever-increasing interest in the refinement and reuse of materials that formerly would have been discarded as waste or junk.

In addition to the kinds of applied research described above, scientists in both fields need to be able to characterize and understand the properties of all kinds of materials under varying environmental conditions. Therefore, basic research on materials and their properties is a fundamental part of the activities of geological and materials scientists, and is probably the area in which common interests can be most easily defined. For example, the study of materials under high pressure is of great interest to both fields. Geological scientists are interested in the elastic properties of minerals at the high pressures within the earth; and materials scientists are interested in super-hard materials synthesized at high pressure, the effect of pressure on solid lubricants, the elastic properties of structural materials under pressure, and so on. The information and techniques resulting from these studies are complementary, and they can be applied to problems ranging across all aspects of the materials cycle and to the initiation of further basic research.

SIGNIFICANCE OF RESEARCH

The activities represented by the materials cycle are obviously essential to any industrialized country; and, because these activities represent an enormous investment and yearly expenditure of funds, even a small improvement in an exploration technique, ore beneficiation, or some other part of the materials cycle can produce a substantial savings of money and an increase in production efficiency. Geological and materials scientists can contribute to many different national scientific and technological objectives, among them the following:

- 1. The indigenous U.S. mineral resource base is shrinking; ways must be found to improve exploration and mining techniques, to advance ore processing technology for low-grade ores, and to find substitutes for elements and compounds in short supply.
- Specialized materials to support advanced types of technology in the electronics and transportation industries will have to be developed.
- 3. Disposal and isolation of radioactive waste is a serious technological and political problem that can be mitigated by the intelligent application of knowledge and experience from gelogical and materials science.
- 4. The accelerated pace of foreign competition in materials processing, special beneficiation and smelting techniques, ceramics, and high-technology areas poses serious problems for U.S. industry, which is hard put to compete successfully because it is bound by more

restrictive rules and regulations than many foreign companies. New foreign technologies can, of course, be purchased under license agreements, but this adds to the costs of domestic products and further hampers U.S. industry.

- 5. The need for synthesis of new materials and improvement of synthesis techniques is a common problem and an area in which much benefit could be derived from cooperative research projects. For example, knowledge generated from solid earth studies may be utilized in the design, development, and characterization of new synthetic materials.
- 6. Research on hazardous materials such as asbestos is badly needed in order to maintain a balance between misuse of potentially hazardous materials and nonuse because of public reaction arising from the lack of reliable information and guidance.
- 7. The understanding of mechanisms of mass and energy transfer in the earth's core, mantle, and crust is very important to geological scientists, and it is an area where the techniques of the materials scientist can be of great value and where the materials scientist can find challenging research problems.
- 8. Characterization of the compositional (e.g., chemical, phase, isotope) changes with depth in the earth is a major component of modern geochemical and geophysical research.
- 9. Particularly important to geophysicists is the definition of temperature distributions, stress field, and strain rate field in all regions of the earth, and the establishment of the mechanical properties (elastic constants, fracture, viscosity, seismic attenuation, flow laws)

of earth materials, especially under conditions like those found in the earth's crust and mantle. There are boundless opportunities for cooperative research in these areas.

- 10. The rheological behavior of minerals and rocks (together with the processes responsible for it) may be applied to furthering the understanding and prediction of physical behavior in metals, ceramics, and composite materials.
- 11. Knowledge of precursory earthquake phenomena derived from impending fracture in rocks (e.g., electrical, seismic) can be applied to the prediction of similar failure in other materials. Conversely, application of other precursory phenomena observed in nonrock materials can add to our understanding of both seismic and aseismic failure in the crust and upper mantle.
- 11. In all of the above, development of new techniques and instruments for characterizing material properties can be of immense value to materials science and technology, and in many instances it can lead to new instruments or processes that further industrial development.

EXAMPLES OF FLOW OF INFORMATION AND TECHNIQUES

Recognition of the close linkages between geological and materials sciences in terms of tools used to characterize natural and synthetic materials has resulted in sharing of common analytical facilities between departments at a few universities and research laboratories. This tendency for sharing of resources will probably increase in the future,

because of the scarcity of funds for capital equipment, the high cost of state-of-the-art analytical facilities, and the vital need for sophisticated, skilled personnel to maintain, operate, and upgrade the facilities. A crucially important by-product of the resource sharing, within and between institutions, is that researchers from different fields are rubbing elbows and raising scientific questions with one another. The resulting interactions create a natural, operational link between geological and materials scientists.

In addition to using common tools and methods to characterize natural and synthetic materials, geological and materials scientists use similar apparatus to conduct experiments. Frequently, the experimental studies are conducted in such a way as to provide, simultaneously, information that can be used to characterize the dynamic response of materials. Experiments are conducted over pressure ranges from hard vacuum to megabars, over temperature ranges from cryogenic to thousands of degrees, and over time intervals from picoseconds to years. We hasten to point out that although all extremes are not attainable simultaneously, they serve to bound the experimental domain open to the scientist involved with both natural and synthetic materials. Advances in experimental techniques and methodologies have resulted from a free flow of ideas and concepts between geological and materials sciences. Although the underlying motivation for experimental research may differ in the two fields -- as, for example, in the case of materials characterization -- there is a common need to resolve questions bearing on the response of materials to changing conditions of the physical surrounding. Classical studies of heterogeneous (phase) equilibria in multicomponent systems, based on Gibbsian thermodynamics, represent a common approach extensively used by both geological and materials scientists. During the past generation, such studies have evolved to the point where they now incorporate concern with kinetics of crystal nucleation and growth. In materials science this combination of considering both equilibrium and nonequilibrium processes has led to the development of glass-ceramics, a higher level of understanding of microstructure in high-strength alloys, and the preparation of new materials of unprecedented purity. Similarly, this approach applied to natural materials has resulted in a vastly increased level of understanding of the evolution of basaltic rocks on the continents, under the oceans, and on the moon.

COMMON AREAS OF RESEARCH

Introduction

Mineral deposits are mined and processed to form the metals, ceramics, and plastics of materials science that are then used by fabrication industries to make the machines and buildings of our complex society. Most of the chemical elements and compounds of use in materials science come from anomalous and unusual concentrations in the earth commonly called mineral deposits. These are often hard to find, and concentrated efforts by geological scientists are required to locate and mine them. Thus copper and plastics come from ore bodies and petroleum reservoirs that are steadily depleted and for which replacements are increasingly difficult to find in the face of steadily escalating demand. Inevitably, new methods of finding and producing ore and oil

deposits involve interactions between the materials and geological sciences. These interactions can be explained in terms of the chemical and physical properties of the substances of mutual concern.

Both geological and materials sciences must draw their basic knowledge of chemical and physical properties from the more fundamental sciences of physics, applied mathematics, and chemistry. From these basic fields have come the essential physical and mathematical models (e.g., the phase rule, thermodynamics, and rate laws). But research on compounds of interest in geological and materials sciences must extend the basic models and data into more practical applications.

The pressure and temperature conditions and the energy requirements for forming copper deposits in the earth are very different from the energy, pressure, and temperature requirements for forming copper bars in the chemical engineering and physical chemistry of materials processing. But in both cases, the thermochemical properties of copper and its compounds form the basis of our understanding. A discussion of thermodynamic theory and the properties of some chemical elements and compounds of interest in each science is given below.

The physical properties of substances depend on their atomic bonding, crystal structure and microstructure, and the time frame of the process being considered. The physical properties of rocks, minerals, and soils (geological sciences) are similar enough to those of metals, glasses, ceramics, and plastics (materials science) that useful interactions between scientists in the two fields can be productive. Information has been exchanged primarily on mechanical and thermal properties, but there is also information on aggregational, electrical, magnetic, and optical properties. These properties are affected by pressure and temperature,

and appropriate theoretical models are available in statistical and quantum mechanics and solid-state physics. A discussion of common features of physical properties of substances of earth and materials sciences is given below.

We note again that materials science is much the larger of the two fields and the more strongly represented in amount of funding, breadth of research, and number of participants. (We include as materials scientists metallurgists, ceramicists, engineers, and polymer scientists, as well as thermochemists, physical chemists, solid-state physicists, and others. Earth scientists include geologists, petrologists, mineralogists, geophysicists, and geochemists, but of these only a small number, as noted elsewhere, are engaged in materials research.) Both groups have contributed to a common reservoir of data on the chemical and physical behavior of materials. The materials include ferrous and nonferrous metals, cements, borate, silicate and chalcogenide glasses, aqueous solutions, oxide and silicate ceramics, synthetic multiple-oxide, sulfide and halide minerals, solid-state electronic devices, fabrics and textiles, and a large selection of glassy and crystalline solid plastics.

Areas of interest and application can be contrasted with regard to

(1) the goals of the endeavors: materials scientists seek to produce a
material with a specific set of properties, whereas earth scientists try
to use the characteristics of natural materials to deduce the history of
the earth and the distribution of valuable materials within it; and (2)
the time frame: materials scientists deal with applications lasting a
few years and often utilizing thermodynamically metastable states (e.g.,
glasses or quenched alloys), whereas earth scientists often deal with
reactions and products representing millions of years, in which

metastability can be recognized only with difficulty. Generally, these factors have resulted in a one-way flow of information from materials to earth sciences, while the many opportunities for counterflow are overlooked.

Thermodynamic Properties

Equations of state involving pressure, temperature, volume, energy, and composition are indispensable in materials science and in geology and geophysics. Thermodynamic data on minerals and solutions are used extensively in extractive metallurgy, in the study of volcanism, and in the study of metamorphic and sedimentary geologic processes. There has been a continuing and valuable cross-exchange of thermodynamic data on chemical elements, oxides, silicates, sulfates, and many other chemical compounds among metallurgists, geologists, ceramicists, chemists, and engineers. Techniques of measuring thermodynamic data on chemical compounds have evolved from chemistry and other materials sciences, but developments have also come from experimental mineralogists and geologists (particularly in high-temperature, high-pressure, water-bearing systems). Some instruments and procedures have been developed jointly by two or more disciplines. In recent years, geophysicists have developed analytical tools and apparatus in high-pressure, high-temperature chemical physics that later transferred to related research problems in materials science.

The laws of thermodynamics and kinetics are used to attack the problems of energy transfer, phase equilibria, and irreversible processes in geologic and materials sciences. The basic need for thermochemical data from calorimetry, solution chemistry, and phase equilibrium research

has been obvious, and scientists in both fields have helped fill the need. The materials for which equations of state and thermodynamic data are needed include gases, liquids, glasses and amorphous materials, and crystals. The fundamental data needed include phase equilibria, involving pressure, temperature, composition and fugacity, kinetics, and molecular and ionic speciation—that is, the whole range of thermochemical and thermophysical data. One particularly evident need is for better descriptions of the characteristics of the phase being studied; for example, a measurement of the heat of solution of a feldspar crystal is of only minimal value unless the degree of structural ordering is specified. Advantages are obvious in sharing the data among scientific disciplines.

One interface between the disciplines is the field of isotope chemistry. Chemists use isotopes as tracers and indicators in chemical reactions and in analytical techniques; biochemists use isotopes as tracers; there are medical applications of radiation; metallurgists employ isotope chemistry in extraction processes and in energy applications; earth scientists use isotopes as natural tracers, as radiometric clocks for the geologic time scale, and as indexes of the progress of natural reactions.

The need to isolate, store, or use the radioactive leftovers from the production of weapons and energy provides a typical opportunity for intercommunication between materials and earth sciences. The wastes start with a high-level of radioactivity, and they are chemical poisons. They create a heat-generating, corrosive local environment in which long-term hazards include not only accidental rupture of the physical containment but the possibility of radioactive degradation of the

containment materials. Even climatic changes that could modify the thermal and/or chemical setting of the isolation site must be considered. This sort of problem demands the collaborative efforts of scientists from all the related fields.

Laboratory synthesis of compounds has been improving, especially in the production of single crystals with specific properties. This technology is very important in the electronics industry, and it is useful in many other fields.

Classical studies of phase equilibria in multicomponent systems represent a common approach extensively used by both earth and materials scientists.

The simpler binary, ternary, and even quaternary systems of interest to materials scientists and geologists have received considerable attention and are generally well understood. Yet even these "simple" systems show complexities beyond the scope of classical phase equilibrium studies. Current emphasis is more on complex and exotic systems and on dealing with less tractable components, such as H2O, HF, S, and others. Moreover, there is a substantial shift toward acquisition and application of thermodynamic data from simple systems as an aid to predicting the behavior of more complex systems. In line with this shift is the rapidly expanding reservoir of information on the properties of solid solutions (especially the spinels, pyroxenes, feldspars, olivines, and sulfides). The whole realm of the quantitative understanding of the thermodynamic properties of hydrous silicate melts has been strongly advanced by the earth science community, as has the difficult area of the physical chemistry of aqueous solutions at temperatures and pressures approaching the supercritical. The latter has immediate application to

understanding of the genesis and distribution of mineral deposits, but it also has potential application to the extraction of metals from ores in a refinery or in situ production through solution mining, and to the interaction between radwaste and the environment.

Physical Properties

Statistical and quantum mechanics provide the theoretical framework for physical properties of solid materials. For the most part, however, each physical property has its own separate body of theory and its own physical and mathematical models. The complexity can be demonstrated by considering mechanical properties. In mechanics the mathematical models include the theories of elasticity, plasticity, dislocations, viscosity, statics, kinematics, and dynamics; experimental results on mechanical properties are the basis for physical models of stress, strain, fatigue, strength, friction, work hardening, dislocation, fracture, creep, and plastic flow. The other physical properties use models in a similarly complicated fashion.

Comparisons can be made between rocks (including minerals and soils) and the various substances in materials science, and similarities and differences in physical properties can be made clear.

The differences in the types of atomic bonding in metals, ceramics, and minerals, i.e., the differing characteristics of metallic, covalent, and ionic bonding, account for many of the differences in their mechanical properties, e.g., ductility, work hardening, viscous strain and relaxation, self-diffusion, and creep. But some properties of metals are directly translatable to rocks; these include elasticity, plasticity, and viscoelasticity. Idealized behavior, according to these theories,

is applicable to rocks under certain ranges of conditions.

Unfortunately, data for rocks are still too sparse to be of much use for metals. The effects of temperature and strain rate in metals are applicable in part to rock behavior. The thermal and optical properties differ widely between metals and rocks; electrical and magnetic properties are similar, especially metals and ore minerals, and the basic models and measurements come from physics. Therefore, because there are some similarities in mechanical properties between rocks and metals, there has been some interaction between research workers. More interaction should be encouraged.

As with metals and rocks, differences in bonding of atoms between glasses and rocks—in this, case amorphous versus covalent—account for many differences in mechanical properties. Glasses below the glass transition temperature are brittle and fail by fracture; some rocks show a similar brittleness, and results learned from glass are applicable in part to rocks. Above the glass transition temperature, the viscous behavior of glass is similar to rock magma. Physical and mathematical models for glasses are useful for rocks, and a concept like the weakening effects of surface cracks carries over nicely. Data and models for thermal, optical, electrical, and magnetic properties of glasses have been useful in rock and mineral studies.

Silicate ceramics are closely similar to rocks in their covalent bonding of silica tetrahedra; and their physical, especially their mechanical, properties are likewise similar. Models and actual property data from ceramics are used commonly in analyzing rock behavior over wide

ranges of temperature (up to 1000°C) and pressure (up to 10 kbar).

Elastic properties and strength are virtually interchangeable, and there have been a number of translations from geological to materials sciences based on studies of hydrolytic weakening of quartz, the onset of microfracturing in compression tests, friction in many types of rocks, and the high-temperature "plasticity" of ferromagnesian silicate minerals. Oxide ceramics are like oxide minerals, and data are easily transferable.

Solids of polymer plastics are organic, nearly homogeneous, and, predictably, they have physical and mechanical properties quite different from those of rocks. Therefore there has been only a limited interchange of data between plastics and natural compounds, mostly the application of polymer models to silicate glasses. Although plastics have a very small elastic range under stress, they do exhibit viscoelasticity; and the models developed for plastics are useful to model ideal viscoelastic behavior for rocks. Compared to rocks, plastics are relatively weak but are like soils in the phenomenon of thixotropy.

Another area of commonality between the materials and geological sciences is the structure and deformation behavior of partially melted systems with low-melt fractions. In ceramics, a great deal of effort has been put into the study of silicon nitride for structural applications in heat engines. Analogous is the partial melting of peridotite in the earth's mantle, which is called upon to explain many phenomena, such as the low-velocity layer, convection and plate tectonics, and the origin of volcanic eruptions of basalt.

Two prominent areas of recent research of interest to both fields are the Brillouin scattering techniques used to obtain single-crystal elastic

constants of extremely small samples, and the measurement of anelastic properties and internal friction of rocks and minerals at seismic frequencies. Collaboration between physicists and geophysicists on solid-state problems should lead to further improvements in techniques.

High-temperature deformation in rocks and minerals correlates with steady state creep in materials science. Mechanisms of plastic deformation of metals and ceramics include dislocation climb and glide, grain matrix diffusion, grain boundary diffusion, and grain boundary sliding. These same processes have been recognized in the flow of minerals. Further research in both materials and earth sciences is needed to explore transient creep, anelastic deformation, and attenuation of waves, and to extrapolate results obtained on a laboratory time scale to the much longer times that are important in engineering applications and in geologic processes.

An interdisciplinary conference on "Mechanisms of Deformation and Fracture," was held in Lulea, Sweden, September 20 to 22, 1978, and the proceedings volume (Easterling, 1979) cites areas of mutual interest among earth sciences, materials science, and solid mechanics. Feltham (Easterling, 1979, pp. 29-41) discusses concepts and models of mechanisms of plastic deformation in earth and materials sciences, including ductile behavior above the glass-transition temperature, the brittle-to-ductile transition, energy-barrier heights, and microstructures in models. Feltham refers particularly to plastic flow in clay. Broberg (Easterling, 1979, pp. 3-28) compares fracture mechanics involved in earthquakes with fracture in engineering structures. In 15 experimental studies and 19 theoretical studies, applications to metals and other

materials and to rocks and soils are described, including interactions among the three sciences.

Other phenomena closely related to and strongly influenced by physical properties include solid-state precipitation (also called exsolution) and phase transformations. Because these are highly dependent on the properties of the surfaces of the constituent, they will be discussed in the following section, on "Surface Studies."

In general, there has been a useful adaptation of chemical, physical, and mathematical models from the materials science to the geological sciences, particularly where the rock and the materials properties are similar. However, there has been less reverse flow of information to materials scientists, probably because rocks and minerals are more complicated and uncontrollable than metals, glasses, ceramics, and plastics.

Surface Studies

Introduction

Surface studies are, in a sense, a subset of physical properties, but they are so important that we will treat them separately.

Surface studies are one of the best examples of the common spine of materials science and geological science. Since 1980, remarkable advances in tools and techniques have enabled scientists and engineers to study the structures and compositions of surfaces. Auger spectroscopy, scanning electron microscopy, field ion microscopy, and low-energy electron diffraction are some of the most important techniques. And even though many of these techniques have been available for many years,

recent advances and refinements have made them far more powerful.

A well-equipped laboratory facility for studying surfaces could easily cost \$1,000,000 for equipment alone. Continuing support is also expensive. It is therefore unlikely that any single university or laboratory could set up separate laboratories for geological and materials sciences. However, the two groups have much to learn from each other, and a combined laboratory would encourage productive interaction. General university courses in diffraction, microscopy, and spectroscopy applied to surface phenomena are perhaps better than courses applied specifically to metals, ceramics, or minerals. The general courses may be not only more economical, but, more important, may also be more stimulating to the student.

The thermodynamics of adsorption, first treated by Gibbs more than 100 years ago, is the same whether one is dealing with a metal, ceramic, polymer, or mineral. Thus, scanning Auger microscopy has recently led to the identification of the nature and concentration of the embrittling segregants along the grain boundaries in metals. And through such studies, metallurgists are learning how to prevent temper embrittlement. The similar segregation that must occur in metamorphic rocks has barely been looked at. Such studies would have great practical importance in rock mechanics—for mining and crushing of rocks and in use of natural structural materials.

Another example of commonality between materials and geological sciences is the phenomenon called solid-state precipitation in metals and exsolution in minerals. Most strong metals are strong because they contain small precipitate particles throughout, formed by nucleation and growth of second-phase particles in a supersaturated solid solution.

Elevated temperature, aging, or heat treating is usually needed to carry out the reaction. But if carried too far, segregation of the exsolved phases becomes significant and strength decreases. The kinetics of nucleation and growth are determined in a large measure by surface energy and surface absorption considerations. Exsolution has occurred in the minerals of rocks that were formed under high temperatures and pressures and then brought to the earth's surface. Exsolution occurs also during weathering and surficial alteration of rocks and minerals. Understanding this process is an important field of geological science. Much is to be gained by researchers on metals and those on minerals working together. In particular, modern surface science techniques put scientists in a better position to place this field on a sounder basis.

Several specific fields will now be discussed in somewhat more detail.

Mineral Beneficiation

Most metal ores being mined today are relatively low grade and must be beneficiated to eliminate the large percentage of worthless rock and mineral that naturally accompanies the ore. This step masquerades in various titles such as ore dressing, mineral dressing, and mineral processing.

It is inevitable that the grade of most metal ores will decline in the coming years. More effective beneficiation will be needed to obtain a sharper separation between the valuable minerals and the waste.

Furthermore, beneficiation processes that can be more selective among several minerals in the same ore will be needed.

Beneficiation is achieved by one or more of several processes, but

particle size must be small enough that the ore minerals are broken away from the worthless rock or that chemical separation is more readily achieved. The intensive grinding necessary to achieve separation both increases the cost and at the same time produces small particles that, although liberated, are not as easily collected as larger ones.

Methods of separation after crushing are based on some difference between the properties of the valuable mineral and the worthless rock. The simplest difference is density, which is of little concern to us in this report, for separation can be achieved with pans, sluices, jigs, shaking tables, and similar devices. Other physical properties used for separation include magnetism and electrostatic phenomena.

Beneficiation processes that involve surface phenomena are flotation and hydrometallurgy. A good example of flotation is the treatment of the copper ore from Bingham Canyon, Utah. Material containing as little as 0.4 percent copper (8 pounds of copper per short ton of ore) and with even less molybdenum can be treated at a profit when the price of copper is reasonably high. The copper in the Bingham ore is mostly in the mineral, chalcopyrite (CuFeS₂), which is approximately 1 wt. percent of the mined material. Thus the problem is to recover the chalcopyrite (1 wt. percent), molybdenite (0.1 percent), and gold (1 ounce per ton) in separate concentrates and to discard the worthless material (99 percent) into tailings. This is accomplished in a flotation mill.

Flotation is the most widely used method of separation. The process usually consists of introducing air bubbles into a pulp of finely ground ore and water. One constituent, usually the valuable mineral, clings to

the bubbles, rises to the surface and is scraped off to make a concentrate. The other constituent, usually the worthless rock, is wetted by the water, does not stick to the bubbles, and is carried away into the tailings. The success of the process depends on the surface of the valuable mineral being hydrophobic (water repellent) so that it will adhere to bubbles, while the surface of the worthless material is hydrophilic (wetted by water) and will not cling to the bubbles.

Very few minerals have natural flotability; only graphite and molybdenite (MoS₂) float without previous treatment. In order to achieve the conditions of a water-repellent surface on one mineral and a water-avid surface on another, reagents are added that change the chemistry of the surfaces only and hence their attraction to air bubbles.

In early days, petroleum oils were the common reagents. These leave a greasy film on the surface of the minerals but do not cling to the silicate rocks. The resulting concentrate contains all of the sulfides, and therefore includes pyrite as well as the ore minerals. Subsequently, more specific reagents were found that were more selective in their action. These reagents, called "collectors," are usually bi-polar; one end is polar and will react with the mineral surface, while the other end of the molecule is a hydrocarbon chain that presents a nonpolar water-repellent surface to the ore-water slurry.

No attempt will be made to describe all the collectors that are used or all the auxiliary reagents, such as activating agents, sulfidizing agents, deactivating reagents, cleansing reagents, depressing reagents, pH regulating agents, and others that make surface chemistry control a sophisticated effort. It suffices to say that as good as these processes

are, there is much room for improvement, and the poorer grades of more complex ores that must be worked in the future will require such improvement. If the knowledge of minerals and their properties now possessed by the geological sciences can be transferred to the materials science, we can look forward to some further improvement of separation processes. A better understanding of surface properties and surface phenomena including adsorption should allow flotation to be placed on a firm scientific footing. On this basis, one might anticipate the sort of quantum jump advance in flotation technology that is occurring in catalysis.

In addition to beneficiation per se, hydrometallurgy includes the physical and chemical processes involved in solution mining, dump or heap leaching, hydrometallurgical extraction, and microbial applications. An important example is the recovery of gold, silver, copper, and nickel by extraction with various aqueous solutions.

Research is needed on basic physical-inorganic chemistry and unit processes, leachant-rock and leachant-ore mineral reactions, and the chemistry of high-ionic-strength solutions: chemical reduction of metals from solutions; solvent extraction and highly selective chelating reagents; interfacial phenomena at aqueous-organic interfaces; chemical transport membranes; bacterial reactions as applied to mineral recovery, desulfurization of coal, and restoration of the environment following resource recovery.

Phase Transformations

The field of phase transformations is another good example of surface phenomena of interest to both materials science and the geological sciences. Phase transformation ordinarily involves formation of a nucleus of the new phase, and the surface energy required is a barrier to such nucleation. Once the new phase has formed, it grows by expansion of its surface, so the properties of the interface between the phases usually govern the rates of transformation. An example is the addition of alloying elements, such as chromium and molybdenum, to steel to increase the hardenability. Similarly, the habit of natural and synthetic crystals is determined by the impurities that segregate to the surfaces of the growing crystals. The role of impurities in hardenability and on the habits of crystals can now be quantitatively studied with modern techniques for characterizing surfaces, but such research is only beginning.

A great deal of both the geological and materials worlds may be characterized by the term "metastable," where we deal with products and processes that are "suspended" in energetically activated states. In such states, phase change is the rule. Given processes operating at finite rates and for infinite time, we would most often observe stable (equilibrium) states; they would achieve this status by grain nucleation, growth and reorientation, transitions to new phases, phase separations from originally homogeneous phases, reactions between phases, grain growth, and so on. In fact, what we usually observe is incomplete attainment of equilibrium or even disequilibrium. Glassy rocks and piano wire are examples of metastable states. The boundaries between grains (i.e., the surfaces) are especially critical to our interpreting the

state of rocks and minerals (the interest of the geoscientist) as well as understanding the processes necessary to produce a desired product (the concern of the materials scientist). Thus rusting is the return of metastable iron to its stable state in air, and we retard this corrosion by introducing a barrier to the chemical reaction at the iron surface.

Likewise, the development of a protective film, such as aluminum oxide on kitchen ware, makes passive a metal surface in a potentially very reactive medium and thereby provides a useful product. Similar processes occur at the surfaces of rocks as they weather to yield soils and to ores as they oxidize and become dissipated through metal migration in groundwater. Thus an understanding of the behavior of surfaces in contact with air or aqueous solutions provides a broad common ground for materials and earth sciences.

In the phenomenon of solid-state precipitation, examination of the thermodynamics shows that there may be several solvus lines. The preferred line depends on the extent to which the crystal structure of the exsolved phase forms coherent or incoherent interfaces with the host. For example, a fluctuation in composition can form within a phase and without the usual nucleation if there is no chemical free energy barrier. This leads to spinodal decomposition, where the composition fluctuations are periodic. Such spinodal decomposition has occurred in minerals such as the feldspars and can be made to occur in metals and ceramics. An example of the latter is the well-known process for making quartz glass.

While much has been done in this field, the surface energies and role

of impurities are only qualitatively known and have been largely inferred indirectly. Materials scientists and geological scientists could now obtain much more quantitative information using Auger analysis and other techniques. This is a research area of great technical and scientific importance.

Impurity Segregation and Fracture

As already mentioned in the introduction, the fracturing of rock is an area that presents considerable opportunity for the application of surface materials science. Fundamentally, the energy required to break bonds within or between crystals can be reduced by segregating (and concentrating) impurities at the surfaces or interfaces. In metals and ceramics, where the phenomenon has been studied using scanning Auger spectroscopy, current research is aimed at understanding and reducing this segregation. For crushing and grinding of ores during mineral beneficiation, propagation of fractures during blasting, hydrofracturing of rock for geothermal energy production, petroleum recovery, solution mining, or similar operations, the opposite effect would be highly beneficial and research would be pointed toward additional segregation. The fracture path in rocks during seismic events may well be related to segregation of impurities. Therefore, researchers studying this phenomenon in metals and ceramics should be encouraged to extend their study to rocks and minerals.

COMMON TOOLS, TECHNIQUES, AND MATERIALS

During the past ten years, members of the geological sciences community have made a serious effort to use a variety of spectroscopic techniques for investigating material properties of rocks and minerals. This effort illustrates how the use of analytical methods developed in other disciplines can advance understanding of geological materials and in turn can help advance the analytical procedures. Spectroscopic studies of rocks and minerals now range from X-rays to infrared and, in scale, from a few microns to square kilometers.

Spectroscopy

X-ray spectroscopy is a key tool in rock and mineral analysis. It became an indispensable microanalytical tool through the advent of the electron microprobe, which combines the focusing capability of an electron microscope with an X-ray spectrometer. The electron microprobe was originally developed outside of the geological sciences, but its use as a quantitative analytical instrument for chemically complex materials came about when geoscientists adopted the instrument and developed procedures for analyzing materials as complex as rocks. Because of these mutual efforts the electron microprobe is now a primary analytical instrument for the study of inhomogeneous solid matter.

Similarly, Mossbauer and optical spectroscopy were developed and employed by physicists and chemists long before they were seriously utilized for problems related to geological materials; but these two methods have proven very useful in studies of mineral properties, addressing problems related to phase identification, cation oxidation states, and aspects of crystal structures. And in turn, geoscientists have advanced these experimental methods, particularly for the study of small anisotropic solids and materials at extremely high pressures.

Vibrational spectroscopy, both infrared and Raman, has also been adopted by geoscientists. Infrared spectra were first used primarily for phase identification. This important application continues and has been refined to the point that only micrograms of material are required. Both infrared and Raman spectra are used in the study of amorphous minerals (glasses and radiation-damaged materials) and very fine-grained minerals (biological mineralization, weathering rinds). Raman spectra are used in studying the structure of glassy rock; and infrared spectra are used to investigate trace amounts of water in minerals, a ubiquitous component of natural systems that affects both physical and chemical properties. Vibrational spectra have also been used to compute thermodynamic properties of minerals, which suggests that it may be possible to compute (rather than measure) these properties for materials that are difficult to obtain in quantity adequate for conventional measurements (e.g., high-pressure phases that are found at depth in this planet).

New spectroscopic methods will certainly be used by geoscientists to enlarge the scope of problems that can be addressed. Two emergent examples illustrate the potential.

The first is X-ray fine structure analysis using synchrotrons as sources of intense radiation. This technique has the potential of identifying concentration, state of oxidation, and the structural

environment for almost every element. No other type of spectroscopy can combine all these features. This research uses large central synchrotron radiation facilities that are currently being expanded. However, much development and experimentation remains before the objectives can be reached. In this area, the new synchrotron, described below, will be of major importance.

The second is solid-state nuclear magnetic resonance, which is being developed to study the concentration, dynamic motion, and structural environment of water molecules in solids. This technique complements infrared spectroscopy by avoiding many of the tedious sample preparation requirements and by responding to the motion of the water molecules on a different time scale. The development of methods for the study of water in rocks and minerals has important applications to an enormous variety of geological processes such as ore deposition, weathering, and volcanism.

Synchrotron Radiation

Probably the most exciting new research tool of recent years is the synchrotron, a machine capable of producing high-intensity electromagnetic radiation for research on materials. Several synchrotrons have been built or are under construction in the United States, Germany, Great Britain, France, the U.S.S.R., and Japan. In the United States, three synchrotron facilities are now in use--at Stanford, Wisconsin, and Cornell universities--and a major new one is nearing completion at Brookhaven National Laboratory. The latter installation is unique in that it is designed for use by a wider range of research workers. Its high-intensity radiation will be available from a number of

beam lines and will range from the X-ray region through the ultraviolet, the visible, and into the infrared. The availability of these radiation sources will permit geological and materials scientists to perform experiments involving the fundamental properties of solids, liquids, and gases that are not possible with conventional radiation sources. The experiments will include investigation of surfaces through X-ray scattering, X-ray diffraction at high temperatures and pressures, the study of atomic coordination through detailed X-ray absorption measurements, and characterization of order-disorder phenomena. The opportunities for collaboration in the design and execution of appropriate experiments are endless and should receive major and immediate attention from geological and materials scientists throughout the United States.

Growth of Single Crystals

Growth of single crystals of high purity is, perhaps, one of the most important activities common to both geological and materials sciences. This activity employs a wide range of environment-controlled, high-temperature furnaces. The choice of furnace depends upon the growth techniques. The materials include various oxides, silicates, and metallic alloys that are analogs of the supposed constituents of the earth's interior.

Geologists have, in the past, depended primarily on materials scientists (ceramicists, crystal chemists, and metallurgists) to grow various types of single crystals for characterization and for physical property measurements. A few can be purchased from supply houses, but

most must be custom grown. Earth science laboratories are not in a position to sustain long-term crystal-growth programs, and the number of laboratories in the United States with long-term programs engaged in growing single crystals of geophysically relevant materials is negligible. In contrast, Japan has several crystal-growth laboratories with long-term commitments by a research group or an institute (e.g., at Tohoku University, at the Tsukuba Institutes, and at the Institute for Researches in Inorganic Materials).

With one or two exceptions, the art and science of crystal growing has not been fully exploited by earth science laboratories in this country, in part because of the lack of commitment to long-term funding and the lack of adequate facilities. Some of the materials science laboratories in the United States have the necessary facilities, but the actual crystals grown in materials science programs are not of much interest to the earth scientist.

High Pressure-Temperature Research

General Statement

Interaction between physicists and geologists in high

pressure-temperature research started in the first decade of this century

with the experiments of Arthur L. Day in Washington, D.C., and of Percy

Bridgman in Cambridge, Massachusetts. (Bridgman won the Nobel Prize for

his research.) Since then, physics and geophysics have interacted

sporadically, primarily at times of breakthrough in technology. Today

the need for interaction is particularly acute, because the two fields

(now called materials science and earth science) have focused on the phenomena at the interface between phases.

The fundamentals are the same in both fields. The materials scientist uses high pressures and temperatures to synthesize new materials or to treat existing ones. The earth scientist uses high pressure and temperature to study earth and planetary materials under the intense conditions of the interiors of the planets. Groups of properties of materials that interest the earth scientist include chemical compositions, mineralogical compositions, equations of state (pressure-temperature-volume-energy), thermal history, dynamic behavior, and magnetic behavior. Among these properties, the following list includes many of the experimental properties of materials sought by both the earth and the materials sciences.

Phase transitions and equilibria (first order, electronic or magnetic) crystal structure oxidation states site occupancy element partitioning CFSE (crystal field stabalization energy) charge transfer reaction kinetics melting solubility diffusion K-capture decay rate density sound velocity elastic moduli thermal expansion Cp or Cv (heat capacity, Gruneisen parameter) phonon modes thermal conductivity electrical conductivity energy gap polarizability index of refraction magnetic properties viscosity strength

In addition to studies of the actual materials and their properties, the technology of high pressure and temperature is also an important interface between the two fields. The main technological areas of development include the following:

- 1. Pressure and temperature generation
- 2. Pressure and temperature calibration
- 3. Degree of hydrostaticity of the pressure field
- Accuracy and precision of pressure and temperature measurement relative to calibration

In situ measurements at high temperature and pressure that are needed by both earth and materials scientists are as follows:

- 1. Electrical measurements
- 2. Magnetic measurements in external fields
- 3. Scattering or reemission
- 4. Diffraction
- 5. Absorption

The last three involve several supporting techniques, as follows:

- Scattering or reemission: Raman, Rayleigh, fluorescence, and black body radiation.
- Diffraction: X-ray, Brillouin, and gamma-ray.
- Absorption: Mossbauer effect, X-ray K absorption edge, UV, VIS, NIR, and IR.

Synthesis of High-Pressure Phases

Synthesis of the high-pressure phases of olivine and pyroxene has, in many instances, led to determination of important physical, elastic, magnetic, electrical, and thermodynamic properties of those phases.

These, in turn, have important implications about the earth's deep mantle. For example, the single-crystal elastic constants of a synthesized specimen of stishovite (rutile form of SiO, stable at

pressures above 100 kbar) and the thermodynamic properties of several high-pressure spinels have recently been measured. There is, however, a continuing need to determine the elastic and thermodynamic properties of the other higher-density (post-spinel) phases that are postulated for the deeper parts of the mantle.

Large-volume multianvil presses have been extensively used by geophysicists, geochemists, and materials scientists in Japan to synthesize high-density phases at conditions of the upper mantle (i.e., at pressures of up to 250 kbar and 1600°C). Samples of sufficiently large size have been synthesized to allow determinations of thermodynamic properties. There is a need for developing such synthesis facilities by the earth and materials sciences in the United States, and along with it is an unusual opportunity for collaborative research in this area.

Physical Characterization and Chemical Composition

Electron microscopy is one of the most powerful tools that has been used by both materials and earth scientists. And, as noted earlier, earth scientists have made valuable contributions in analytical techniques of instruments developed by other fields, notably the electron microprobe, scanning electron microscopy (SEM), and transmission electron microscopy (TEM). As noted in the section on surface phenomena, probe techniques originally developed for metals are now being extended by earth scientists analyzing complex silicate minerals. Here the geologist's experience with complex silicates is being transferred back to materials science. Other common tools used for characterizing materials and for determining chemical composition are X-ray and

gamma-ray methods (e.g., diffraction, scattering, fluorescence, EXAFS, and Mossbauer effect), Raman spectroscopy, and radiometric methods.

Special types of high-energy sources being developed and employed by both groups of scientists are synchrotron sources (for diffraction and EXAFS studies) and neutron sources (for neutron diffraction and scattering studies). But much of the development is being achieved separately. Cooperation between the earth and materials scientists saves both groups time, effort, and money in the few instances where it takes place; increased cooperation would yield commensurate savings.

Materials

Materials researchers and earth scientists share the need for samples of crystalline, polycrystalline, and glassy materials for study.

Materials scientists' requirements, while normally encompassing a simpler compositional range, often extend to higher levels of purity or more specific impurity than do those of the earth scientists. The earth scientist must deal with complex, frequently nonstoichiometric, mineral compounds (natural as well as synthetic). In the limited cases where it has occurred, cross-disciplinary flow and exchange of ideas have been advantageous. For example, there has been the transfer of knowledge gained from synthesis, chemical analysis, and characterization by earth scientists of materials with complicated structures and compositions, whereas the materials scientists have advanced techniques to determine physical properties. Furthermore, both disciplines have benefited from the exchange of computer software systems for data reduction and for instrument automation.

The number of mineral and other compositionally complex substances whose physical properties are well characterized decreases rapidly as a function of the degree of intensity of pressure-temperature conditions needed to stabilize them. In the high-pressure ranges, for example, the number of stable phases decreases, but the difficulty in studying the materials increases.

Compounds studied by both earth and materials scientists include metals, metal oxides, sulfides, and silicates. Although individual aims differ, the basic objectives of the two disciplines are the same. Both disciplines need to know the major and minor element chemistry of condensed phases and mineral substances. Both need to determine the effects of impurities or trace elements. And both need to characterize materials chemically, physically, and thermodynamically. The equation of state of hydrogen, for example, may form the basis of predicting under what conditions it might be transformed into a metal. And the fundamental properties of hydrogen and helium in their metallic state could form the basis for predicting the properties of an alloy. The earth scientist, in the same context, needs identical data to predict the properties of the cores of planets, including the earth's.

Data on the properties of oxide, silicate, and sulfide compounds have been and are being exchanged between the earth and materials sciences, but the need for increasing this interchange becomes more critical as the levels of sophistication in research rise. There is a strong parallel, for example, between the work of solution geochemists and that of metallurgists. The geochemists examine the process of hydrothermal solutions in nature; the metallurgists use hydrometallurgical techniques

for the solvent extraction of metals from ores. The processes are similar. A direct bridge between the two disciplines exists where hydrometallurgy is applied directly to extract metals from ores in the ground, but the interchange of ideas could be greatly improved.

An Example in Brief

Diamonds have long inspired in man awe, admiration, and covetousness. The high-pressure phase of carbon, diamond is the hardest known natural substance, and it has a very high refractive index, properties that have long made it a prized gemstone. More recently, largely within this century, the hardness of diamond has led to multiple industrial uses, primarily as an abrasive. And since World War II, industrial grade diamonds have been synthesized by a number of experimenters.

But diamond, the mineral, is also of great interest to both the geologist and the materials scientist. The geologist studies diamonds because they form at great depths in the earth. Therefore the diamonds and the numerous impurities found in them-garnets, pyroxenes, olivenes, micas, etc.—tell much about the chemical and physical environment of the earth's mantle. Around the inclusions are areas of stored strain, whose patterns can be deconvoluted by theoretical analysis to determine the state of stress.

The materials scientist studies the physics of diamonds for a variety of reasons that have recently been described in some detail by Davis (1981) of the Wheatstone Physics Laboratory. Davis notes that diamond represents the extreme covalent form of crystalline bonding better than

the more easily synthesized silicon with diamond structure. Diamond's transparency is employed in numerous optical studies that range into the ultraviolet to probe equally the ground and excited states. Diamond has a high Debye temperature, and thus measurements can be made at relatively warm (liquid nitrogen) conditions. The properties of diamond were studied and reported on by pioneers such as Raman and others for these reasons, but, as Davis states, very few experiments have been done to control the impurities in diamonds.

Finally, diamond is the strongest as well as the hardest material on the earth, a property of interest to both the geophysicist and the materials scientist. A pure diamond is probably the strongest possible substance for use as pistons in high-pressure apparatus, but its strength can be greatly reduced by impurities or other imperfections.

Yet despite the scientific importance of and interest in diamonds, diamond synthesis is dominated by marketing applications. There is essentially no program in the United States to synthesize diamonds with specific properties, and no program to investigate how to enhance the desirable qualities and eliminate or minimize the undesirable.

Thus, even such a comparatively well-known substance as diamond could profitably be the target of joint research by earth and materials scientists.

Examples of other crystals of interest to both geological and solid-state science abound. Noncrystalline materials, such as glasses and amorphous substances, are of equally high fascination to scientists of both disciplines.

INSTITUTIONAL AND FUNDING PROBLEMS

Although the geological and materials science communities are aware of each other and do collaborate from time to time, their organizational separation in virtually all institutions is a powerful barrier to interaction and collaboration between the two fields. Few universities have materials science laboratory facilities that are used by geologists, and still fewer have geology departments with X-ray diffraction or electron microprobe facilities that are used by materials scientists.

The exceptions are easily identified. Geology departments are usually in Colleges of Arts and Sciences; materials science departments in Colleges of Engineering. This division virtually guarantees that overlaps in curricula and cooperative programs will be minimized. Not only is cooperation difficult, but there is virtually no common experience for geological and materials science students.

The same separation carries over to funding agencies such as the National Science Foundation and the Department of Energy, where the two fields are covered by different offices and staffed by people with different educational backgrounds. This situation poses an even more formidable barrier to cooperation. Program managers say that they are willing to consider interdisciplinary proposals, and they do. At NSF in particular there has been considerable cooperation and some joint funding between the Divisions of Earth Sciences and Materials Science. In the main, however, cross-disciplinary proposals are usually funded, if at all, by only one office. Program managers do not commonly seek joint support from other program managers, because they anticipate requests for

reciprocal support in the future. The results would be a zero-sum activity that would only cause administrative troubles for the managers. And consideration of interdisciplinary proposals by only one of the constituent disciplines mitigates against success of the proposal. The reviewers and staff naturally take the point of view that, although the science may be good, budgets are limited and priority should go to proposals whose major thrust is in their particular discipline.

Returning to the universities, we find also a parochialism that tends to inhibit the development of interdisciplinary programs. The geological profession has traditionally been field-oriented; and in the past, most geologists were involved in geological mapping, mineral exploration, and the study of various kinds of phenomena on the earth's surface. In recent years, laboratory-based research has become increasingly important; and, as a result, students and faculty are faced with a broad range of options. Most departments understandably require that students be familiar with a large portion of this range, but this leaves no time to explore other opportunities in departments such as materials science. This problem is particularly acute in geology departments where there is rivalry or competition between the "field-oriented" and "laboratory-oriented" faculty members. A geology student who wants to concentrate on some aspect of materials science must be careful that he can answer questions on deposition of carbonates or seafloor spreading in order to pass general examinations, even though time spent learning quantum mechanics might be more useful in his research. But the problem is not only with geology. The materials science departments too have full curricula, and they rarely encourage a student to sample the

possibility of research on the products of nature that are being studied across the campus.

The committee believes that these organizational barriers are probably the biggest obstacle in the path of increased cooperation between the geological and materials sciences. Their removal would open many new avenues. The barriers will have to be examined and addressed at each university and each funding agency. But there is a version of the golden rule that quips that he who has the gold makes the rule, and it is likely that a solution by a funding agency would quickly be reflected at the universities.

CONCLUSIONS AND RECOMMENDATIONS

There is no sharp division between geological and materials scientists; on the contrary, a continuum of interests exists that forms a natural basis for cooperation between the two groups. The primary conclusion of this study is that, although there is now some collaboration between geological and materials scientists, it is limited to only a few institutions, and many more opportunities for fruitful collaboration are being neglected. Greater cooperation could be stimulated through appropriate organizational and financial encouragement.

The potential benefits of increased cooperation are several:

- A. Geological scientists would learn about new theories,
 techniques, and equipment that have been developed by the
 considerably larger, and better financed, materials science
 community. In turn, materials scientists would learn about
 theories and techniques where geologists have made significant
 advances in studying complex natural materials.
- B. Materials scientists would be introduced to important problems related to the mineral industry that can be solved only through an integrated effort among a number of different scientific disciplines.
- C. Although a successful cooperative program would require some additional funding at the start, the benefits would result in a better return on the investment and a more efficient use of money in the long run. A program for increased cooperation should identify and publicize important areas for research that

are now neglected either because of inadequate funding or because of limited communication between those with the problems and those with the means of funding solutions.

The committee strongly believes that increased cooperation between the fields of geological and materials sciences will result in scientific advancement, increased productivity, and more effective use of its resources by the United States in the years ahead. To help achieve this increased cooperation, the committee recommends as follows:

- A. A major effort should be made to emphasize research on mineral resources. These resources are vital to the nation's interests, and both the geological and materials sciences can make significant contributions to their more effective use. The effort could range from providing new support to existing institutions, such as the regional laboratories of the Bureau of Mines and the Geological Survey, to the establishment of new national or regional facilities connected with academic institutions. The scope should range from exploration, through recovery, to processing, and it should involve collaboration between the two fields.
- B. Federal agencies supporting research in geological and material sciences should provide funds for and encourage scientists to submit sound interdisciplinary proposals that combine personnel and facilities from both areas. Such proposals will probably require some organizational changes, because it is difficult for program directors to support proposals of this type. But we believe that little progress towards collaboration will be made

until investigators perceive that interdisciplinary proposals have a reasonable chance of being funded. We suggest that the National Science Foundation establish a pilot program to fund joint projects between investigators in the geological and materials sciences. This program should be funded at about \$1,000,000 per year for five years and should probably be administered jointly by the Divisions of Earth Sciences and Materials Science. Information gained from the administration of this program should then be made available to other agencies that might initiate similar projects appropriate to their missions.

- C. A fellowship program should be organized, preferably with funds from both government and industry, that would allow investigators from one discipline to work in the laboratories of the other. Time periods should range from a few months to a year or more. Such a program would be particularly beneficial to academic personnel who want and need experience in laboratories other than their own.
- D. Professional societies and journals should be encouraged to sponsor symposia, special sessions and meetings, and special issues that illustrate the benefits to be derived from increased cooperation. Such activities already exist to a limited extent; further encouragement with modest funding could produce significant results.

E. Inadequate supply of scientific manpower will be a serious problem in the 1980s; shortages were being felt before the current recession, particularly in the petroleum industry and in the engineering aspects of materials science. These will recur after the economy improves. Furthermore, academic institutions, faced with ever-tightening finances, are having difficulty in competing with industry for trained personnel, a situation that will result in fewer qualified university graduates in the future. On the other hand, students are not aware of the opportunities that already exist along the interface between geology and materials science. And the universities, industry, and government have not done a good job in defining their needs or in communicating with each other to explore and expand programs of mutual interest. We recommend, therefore, that the National Research Council consider establishing a small permanent committee with the objective of overseeing and promoting the kinds of interactions that have been discussed in this report.

REFERENCES

- Davis, G. (1981) The Jahn-Teller effect and vibronic coupling at deep levels in diamond, Reports on Progress in Physics 44, 787-830.
- Easterling, K.E., Ed. (1979) Mechanisms of deformation and fracture, Proc. Interdisciplinary Conf. Lulea, Sweden, 20-22 Sept. 1978, Pergamon Press, New York, 422 pp.